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VOLUME II

FINAL REPORT FOR
CONTRACT NO. CPA-22-69-138

A THEORETICAL DESCRIPTION OF THE LIMESTONE INJECTION - WET SCRUBBING PROCESS

To:

NATIONAL AIR POLLUTION CONTROL ADMINISTRATION
DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE
5710 Wooster Pike
Cincinnati, Ohio 45227
Attention Mr. J. L. Phillips

9 June 1970

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APPENDIX A

ALTERNATE SCRUBBER MODELS

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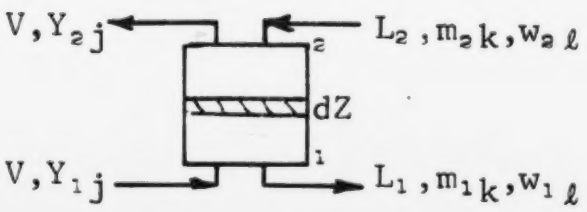
SCRUBBER MODEL - COUNTERCURRENT CONTACTING



Gas Flow: Plug
Liquid Flow: Plug
Solid Flow: Plug
Assume: V is constant

A. GAS-LIQUID RATES

$$-VdY_j = k_{G_j} aSP\left(y-y_i\right)_j dZ \qquad \text{(A-1a)}$$

or

$$-VdY_j = K_{G_j} aSP\left(y-y^*\right)_j dZ \qquad \text{(A-1b)}$$

B. LIQUID RATES

$$-d\left(Lm_k\right) = \sum_n r_{nk} dZ \qquad \text{(A-2)}$$

C. SOLID-LIQUID RATES

$$-d\left(Lw_\ell\right) = \sum_n r_{n\ell} dZ \qquad \text{(A-3)}$$

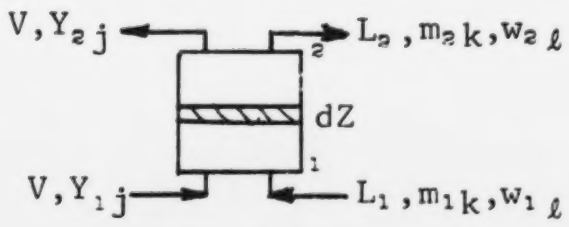
D. MATERIAL BALANCE

$$VdY_j = \sum_k d\left(Lm_k\right) + \sum_\ell d\left(Lw_\ell\right) \qquad \text{(A-4)}$$

NOTE: In general, $r_n = k_n\left[f_{n1}\left(a_{m's}\right) - f_{n2}\left(a_{m's}\right)/K_n\right]$ (A-5)

COMMENTS: This model involves a set of coupled, ordinary differential equations of first order. The number of differential equations could easily be in the 20 to 30 range. With appropriate simplifying assumptions this number could be reduced to around 5 to 10. The rate forms need to be specified and concentrations must be expressed in common terms. Numerical solution on the computer would be necessary.

SCRUBBER MODEL - COCURRENT CONTACTING



Gas Flow: Plug
Liquid Flow: Plug
Solid Flow: Same as liquid
Assume: V is constant

A. GAS-LIQUID RATES

$$-VdY_j = k_{G\,j} aSP\left(y-y_i\right)_j dZ \qquad \text{(A-6a)}$$

or

$$-VdY_j = K_{G\,j} aSP\left(y-y^*\right)_j dZ \qquad \text{(A-6b)}$$

B. LIQUID RATES

$$d\left(Lm_k\right) = \sum_r r_{nk} dZ \qquad \text{(A-7)}$$

C. SOLID-LIQUID RATES

$$d\left(Lw_\ell\right) = \sum_n r_{n\ell} dZ \qquad \text{(A-8)}$$

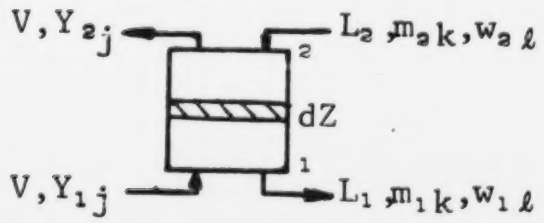
D. MATERIAL BALANCE

$$-VdY_j = \sum_k d\left(Lm_k\right) + \sum_\ell d\left(Lw_\ell\right) \qquad \text{(A-9)}$$

NOTE: In general, $r_n = k_n\left[f_{n1}\left(a_{m's}\right) - f_{n2}\left(a_{m's}\right)/K_n\right]$ (A-10)

COMMENTS: This model involves a set of coupled, ordinary differential equations of first order. The number of differential equations could easily be in the 20 to 30 range. With appropriate simplifying assumptions this number could be reduced to 5 to 10 range. The rate forms need to be specified and concentrations must be expressed in common terms. Numerical solution on the computer would be necessary.

SCRUBBER MODEL - DISPERSED-LIQUID CONTACTING



Gas Flow: Plug
Liquid Flow: Dispersed
Solid Flow: Same as liquid
Assume: V is constant

A. GAS-LIQUID RATES

$$-VdY_j = k_{G_j} aSP\left(y-y_i\right)_j dZ \qquad \text{(A-11a)}$$

or

$$-VdY_j = K_{G_j} aSP\left(y-y^*\right)_j dZ \qquad \text{(A-11b)}$$

B. LIQUID RATES

$$-d\left(Lm_k\right) = \left(\sum_n r_{nk}\right)dZ + \hat{\rho}SD_L\left(\frac{d^2 m_k}{dZ^2}\right)dZ \qquad \text{(A-12)}$$

C. SOLID-LIQUID RATES

$$-d\left(Lw_\ell\right) = \left(\sum_n \bar{r}_{n\ell}\right)dZ + \hat{\rho}SD_s\left(\frac{d^2 w_\ell}{dZ^2}\right)dZ \qquad \text{(A-13)}$$

D. MATERIAL BALANCE

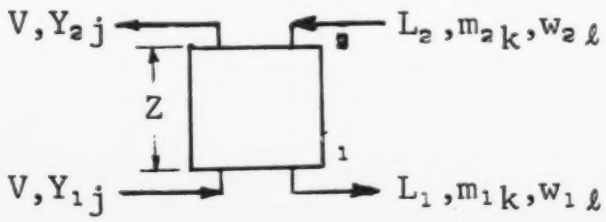
$$VdY_j = \sum_k d\left(Lm_k\right) + \sum_\ell d\left(Lw_\ell\right) \qquad \text{(A-14)}$$

NOTE: In general, $r_n = k_n\left[f_{n_1}\left(a_m\text{'s}\right) - f_{n_2}\left(a_m\text{'s}\right)/K_n\right]$ (A-15)

$$\bar{r}_n = \int_0^{t_s} r_n(t/\tau)dt \qquad \text{(A-16)}$$

COMMENTS: This model involves a set of coupled, ordinary differential equations of second order. The number of differential equations could easily be in the 20 to 30 range. With appropriate simplifying assumptions this number could be reduced to around 5 to 10. The rate forms need to be specified and concentrations must be expressed in common terms. Numerical solution on the computer would be necessary and difficult.

SCRUBBER MODEL - COMPLETELY-BACKMIXED CONTACTING



Gas Flow: Backmixed
Liquid Flow: Backmixed
Solid Flow: Same as liquid
Assume: V is constant

A. GAS-LIQUID RATES

$$V\left(Y_1 - Y_2\right)_j = k_{g\,j}aSP\left(y_2 - y_1\right)_j Z \qquad \text{(A-17a)}$$

or

$$V\left(Y_1 - Y_2\right)_j = K_{g\,j}aSP\left(y_2 - y^*\right)_j Z \qquad \text{(A-17b)}$$

B. LIQUID RATES

$$L_1 m_{1k} - L_2 m_{2k} = \left(\sum_n r_{nk}\right)Z \qquad \text{(A-18)}$$

C. SOLID-LIQUID RATES

$$L_1 w_{1\ell} - L_2 w_{2\ell} = \left(\sum_n \bar{r}_{n\ell}\right)Z \qquad \text{(A-19)}$$

D. MATERIAL BALANCE

$$V\left(Y_1 - Y_2\right)_j = \sum_k\left(L_1 m_{1k} - L_2 m_{2k}\right) + \sum_\ell\left(L_1 w_{1\ell} - L_2 w_{2\ell}\right) \qquad \text{(A-20)}$$

NOTE: In general, $r_n = k_n\left[f_{n1}\left(a_{m's}\right) - f_{n2}\left(a_{m's}\right)/K_n\right]$ (A-21)

$$\bar{r}_n = \int_o^{t_s} r_n R\left(t/\tau\right)dt \qquad \text{(A-22)}$$

COMMENTS: This model involves a set of 20 to 30 algebraic equations. With appropriate simplifying assumptions this number could be reduced to around 5 to 10. The rate forms need to be specified and concentrations must be expressed in common terms. An analytical solution may be possible.

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APPENDIX B

COMPUTER PRINTOUTS GIVING COMPOSITIONS FOR SELECTED PROCESS SIMULATIONS

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PROTOTYPE SIMULATION PS#1-FB

INPUT CONCENTRATIONS (MOLE/LITER)

SO4-- =1.10413+01 NO3- =8.17984-01 CA++ =3.18686+01 MG++ =0.00000
NA+ =0.00000 CL- =0.00000
SO2 =1.10414+01
CO2 =9.81486-01

FILTER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT	
H+	5.492-12	6.111-12	1.113+00	
OH-	1.133-02	8.961-03	7.912-01	
HSO3-	2.155-10	1.705-10	7.912-01	
SO3--	3.035-06	1.189-06	3.918-01	50°C
SO4--	5.797-03	4.747-04	8.189-02	130% theo. LS
HCO3-	2.973-09	2.321-09	7.912-01	0 mole% MgO in LS
CO3--	6.532-08	2.559-08	3.918-01	90% SO_2 removal
NO3-	7.171-01	2.602-01	3.628-01	50% SO_2 oxidation
HSO4-	7.574-13	5.992-13	7.912-01	No fly ash and soluble
H2SO3	1.107-19	1.331-19	1.203+00	Na and CL
H2CO3	2.287-14	2.751-14	1.203+00	
CA++	3.095-01	7.065-02	2.290-01	
CAOH+	2.230-02	1.764-02	7.912-01	
CASO3	2.360-04	2.839-04	1.203+00	
CACO3	3.170-06	3.812-06	1.203+00	
CAHCO3+	4.511-09	3.569-09	7.912-01	
CASO4	7.897-03	9.497-03	1.203+00	
CANO3+	1.007-01	7.970-02	7.912-01	
CACO3(S)	9.815-01	9.815-01	1.000+00	
CASO4(S)	1.103+01	1.103+01	1.000+00	
CASO3(S)	1.104+01	1.104+01	1.000+00	
CA(OH)2(S)	8.379+00	8.379+00	1.000+00	

PSO2 =2.47944-19 ATM.
PCO2 =1.47359-12 ATM.

PH = 11.214 IONIC STRENGTH = 1.[illegible]37+00 RES. E.N. = 8.493-06

PROTOTYPE SIMULATION PS#1-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--=4.41671-02 NO3- =8.17661-01 CA++ =4.79801-01 MG++ =0.00000
NA+ =0.00000 CL- =0.00000
SO2 =3.07533-02
PCO2 =1.43188-01 ATM.

SCRUBBER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT	
H+	1.889-04	2.103-04	1.113+00	
OH-	3.292-10	2.605-10	7.912-01	
HSO3-	7.251-03	5.737-03	7.912-01	
SO3--	2.968-06	1.163-06	3.919-01	50°C
SO4--	5.673-03	4.645-04	8.187-02	130% theo. LS
HCO3-	8.286-06	6.556-06	7.912-01	0 mole% MgO in LS
CO3--	5.363-12	2.102-12	3.919-01	90% SO_2 removal
NO3-	7.150-01	2.594-01	3.628-01	50% SO_2 oxidation
HSO4-	2.549-05	2.017-05	7.912-01	No fly ash and soluble
H2SO3	1.280-04	1.540-04	1.203+00	Na and Cl
H2CO3	2.223-03	2.673-03	1.203+00	10 gpm/ft² SF
CA++	3.154-01	7.233-02	2.290-01	3.74 gpm/ft² SR
CAOH+	6.627-10	5.244-10	7.912-01	15% LS dissolves in S
CASO3	2.360-04	2.838-04	1.203+00	
CACO3	2.661-10	3.200-10	1.203+00	
CAHCO3+	1.303-05	1.031-05	7.912-01	
CASO4	7.899-03	9.500-03	1.203+00	
CANO3+	1.027-01	8.123-02	7.912-01	
CACO3(S)	1.214-37	1.214-37	1.000+00	
CASO4(S)	3.057-02	3.057-02	1.000+00	
CASO3(S)	2.314-02	2.314-02	1.000+00	
CA(OH)2(S)	1.214-37	1.214-37	1.000+00	

PCO2 =2.36943-04 ATM.
O2 =2.24393-03

PH = 3.677 IONIC STRENGTH = 1.[illegible] MSS. T.N. = -7.736-07

PROTOTYPE SIMULATION PS#4-FB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=6.42881+00	NO3-	=4.76208-01	CA++	=1.85767+01	MG++	=0.00000
NA+	=2.75482-01	CL-	=1.84818-01				
SO2	=6.42881+00						
CO2	=3.78062-01						

FILTER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	4.399-12	4.443-12	1.010+00
OH-	1.633-02	1.232-02	7.545-01
HSO3-	3.102-10	2.340-10	7.545-01
SO3--	6.925-06	2.244-06	3.241-01
SO4--	9.404-03	8.960-04	9.527-02
HCO3-	4.221-09	3.185-09	7.545-01
CO3--	1.490-07	4.830-08	3.241-01
NO3-	4.278-01	1.734-01	4.054-01
HSO4-	1.090-12	8.223-13	7.545-01
H2SO3	1.149-19	1.328-19	1.155+00
H2CO3	2.373-14	2.742-14	1.155+00
CA++	1.661-01	3.743-02	2.253-01
CAOH+	1.704-02	1.286-02	7.545-01
CASO3	2.457-04	2.839-04	1.155+00
CACO3	3.300-06	3.812-06	1.155+00
CAHCO3+	3.439-09	2.595-09	7.545-01
CASO4	8.221-03	9.497-03	1.155+00
CANO3+	3.731-02	2.815-02	7.545-01
CACO3(S)	3.781-01	3.781-01	1.000+00
CASO4(S)	6.410+00	6.410+00	1.000+00
CASO3(S)	6.429+00	6.429+00	1.000+00
CA(OH)2(S)	5.131+00	5.131+00	1.000+00
NA+	2.625-01	1.861-01	7.090-01
NAOH	5.343-04	6.173-04	1.155+00
NACO3-	2.644-07	1.995-07	7.545-01
NAHCO3	2.885-10	3.332-10	1.155+00
NASO4-	1.341-03	1.012-03	7.545-01
NANO3	1.112-02	1.285-02	1.155+00
CL-	1.948-01	1.113-01	6.022-01

50°C
130% theo LS
0 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
Fly ash and soluble
Na and Cl included

PSO2 =2.47407-13 ATM.
PCO2 =1.46870-12 ATM.

PH = 11.352 IONIC STRENGTH = 8.24635-01 RES. E.N. = 1.774-08

PROTOTYPE SIMULATION PS#4A-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=4.72442-02	NO3-	=4.76073-01	CA++	=2.63260-01	MG++	=0.00000
NA+	=2.74713-01	CL-	=1.84302-01				
SO2	=2.86187-02						
PCO2	=1.43226-01 ATM.						

SCRUBBER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	1.518-04	1.531-04	1.008+00
OH-	4.745-10	3.578-10	7.539-01
HSO3-	1.044-02	7.868-03	7.539-01
SO3--	6.779-06	2.190-06	3.231-01
SO4--	9.150-03	8.744-04	9.557-02
HCO3-	1.196-05	9.015-06	7.539-01
CO3--	1.229-11	3.970-12	3.231-01
NO3-	4.267-01	1.734-01	4.063-01
HSO4-	3.667-05	2.765-05	7.539-01
H2SO3	1.332-04	1.538-04	1.154+00
H2CO3	2.316-03	2.674-03	1.154+00
CA++	1.702-01	3.835-02	2.253-01
CAOH+	5.072-10	3.824-10	7.539-01
CASO3	2.459-04	2.839-04	1.154+00
CACO3	2.780-10	3.210-10	1.154+00
CAHCO3+	9.993-06	7.527-06	7.539-01
CASO4	8.226-03	9.496-03	1.154+00
CANO3+	3.824-02	2.883-02	7.539-01
CACO3(S)	5.461-33	5.461-33	1.000+00
CASO4(S)	2.852-02	2.852-02	1.000+00
CASO3(S)	1.780-02	1.780-02	1.000+00
CA(OH)2(S)	1.216-37	1.216-37	1.000+00
NA+	2.623-01	1.859-01	7.089-01
NAOH	1.551-11	1.791-11	1.154+00
NACO3-	2.173-11	1.638-11	7.539-01
NAHCO3	8.166-07	9.426-07	1.154+00
NASO4-	1.309-03	9.869-04	7.539-01
NANO3	1.112-02	1.283-02	1.154+00
CL-	1.843-01	1.111-01	6.026-01

PSO2 =2.36535-04 ATM.
CO2 =2.33899-03

50%C
130% theo. LS
0 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
Fly ash and soluble Na and Cl included
10 gpm/ft²
3.27 gpm/ft² SR
15% LS dissolves in S

PH = 3.815 IONIC STRENGTH = 8.20503-01 RES. E.N. = -5.331-11

PROTOTYPE SIMULATION PS#4B-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--=3.78782-02 NO3- =4.75113-01 CA++ =2.44253-01 MG++ =0.00000
NA+ =2.74279-01 CL- =1.84011-01
SO2 =1.92180-02
PCO2 =1.43188-01 ATM.

SCRUBBER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	1.469-04	1.480-04	1.008+00
OH-	4.909-10	3.700-10	7.537-01
HSO3-	1.012-02	7.628-03	7.537-01
SO3--	6.807-06	2.196-06	3.227-01
SO4--	9.160-03	8.766-04	9.570-02
HCO3-	1.235-05	9.311-06	7.537-01
CO3--	1.314-11	4.239-12	3.227-01
NO3-	4.259-01	1.732-01	4.066-01
HSO4-	3.556-05	2.680-05	7.537-01
H2SO3	1.249-04	1.442-04	1.154+00
H2CO3	2.316-03	2.673-03	1.154+00
CA++	1.698-01	3.825-02	2.253-01
CAOH+	5.234-10	3.944-10	7.537-01
CASO3	2.460-04	2.839-04	1.154+00
CACO3	2.963-10	3.419-10	1.154+00
CAHCO3+	1.029-05	7.754-06	7.537-01
CASO4	8.229-03	9.496-03	1.154+00
CANO3+	3.912-02	2.873-02	7.537-01
CACO3(S)	1.217-37	1.217-37	1.000+00
CASO4(S)	1.914-02	1.914-02	1.000+00
CASO3(S)	8.719-03	8.719-03	1.000+00
CA(OH)2(S)	1.217-37	1.217-37	1.000+00
NA+	2.619-01	1.856-01	7.089-01
NAOH	1.602-11	1.849-11	1.154+00
NACO3-	2.318-11	1.747-11	7.537-01
NAHCO3	8.422-07	9.720-07	1.154+00
NASO4-	1.311-03	9.878-04	7.537-01
NANO3	1.109-02	1.280-02	1.154+00
CL-	1.840-01	1.109-01	6.027-01

50°C
130% theo. LS
0 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
Fly ash and soluble Na and Cl included
10 gpm/ft² SF
0 gpm/ft² SR
30% LS dissolves in S

PSO2 =2.68642-04 ATM.
CO2 =2.33983-03

PH = 3.830 IONIC STRENGTH = 8.18689-01 RES. E.N. = 9.652-07

PROTOTYPE SIMULATION BS#4C-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--=3.37037-02 NO3- =4.89955-01 CA++ =2.41269-01 MG++ =0.00000
NA+ =2.82918-01 CL- =1.89806-01
SO2 =1.44449-02
PCO2 =1.43188-01 ATM.

SCRUBBER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	1.508-04	1.534-04	1.017+00
OH-	4.715-10	3.569-10	7.569-01
HSO3-	1.018-02	7.705-03	7.569-01
SO3--	6.520-06	2.140-06	3.282-01
SO4--	9.082-03	3.545-04	3.409-02
HCO3-	1.197-05	9.981-06	7.569-01
CO3--	1.202-11	3.944-12	3.282-01
NO3-	4.387-01	1.763-01	4.019-01
HSO4-	3.578-05	2.708-05	7.569-01
H2SO3	1.303-04	1.510-04	1.159+00
H2CO3	2.307-03	2.677-03	1.159+00
CA++	1.742-01	3.926-02	2.254-01
CAOH+	5.159-10	3.905-10	7.569-01
CASO3	2.450-04	2.839-04	1.159+00
CACO3	2.818-10	3.265-10	1.159+00
CAHCO3+	1.014-05	7.676-06	7.569-01
CASO4	8.199-03	9.500-03	1.159+00
CANO3+	3.956-02	3.002-02	7.569-01
CACO3(S)	1.216-37	1.216-37	1.000+00
CASO4(S)	1.507-02	1.507-02	1.000+00
CASO3(S)	3.883-03	3.883-03	1.000+00
CA(OH)2(S)	1.216-37	1.216-37	1.000+00
NA+	2.700-01	1.915-01	7.092-01
NAOH	1.597-11	1.839-11	1.159+00
NACO3-	2.215-11	1.676-11	7.569-01
NAHCO3	8.346-07	9.670-07	1.159+00
NASO4-	1.312-03	9.932-04	7.569-01
NANO3	1.160-02	1.344-02	1.159+00
CL-	1.893-01	1.140-01	6.008-01

PSO2 =2.11095-04 ATM.
CO2 =2.32995-03

50°C
130% theo. LS
0 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
Fly ash and soluble
Na and Cl included
13.75 gpm/ft² SF
0 gpm/ft² SR
15% LS dissolves in S

PH = 3.814 IONIC STRENGTH = 1.41519-01 RES. E.N. = -3.03[illegible]-02

PROTOTYPE SIMULATION PS#6-FB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=6.65918+00	NO3-	=4.93272-01	CA++	=9.61858+00
NA+	=2.85044-01	CL-	=1.91649-01	MG++	=9.82771+00
SO2	=6.65918+00				
CO2	=5.91942-01				

FILTER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	8.671-09	1.758-09	2.027+00
OH-	2.733-06	3.115-06	1.140+00
HSO3-	1.651-05	1.882-05	1.140+00
SO3--	2.791-05	4.562-05	1.689+00
SO4--	3.632-01	1.821-02	5.014-02
HCO3-	2.247-04	2.561-04	1.140+00
CO3--	5.814-07	9.818-07	1.689+00
NO3-	4.868-01	1.060-01	2.178-01
HSO4-	5.801-08	6.613-08	1.140+00
H2SO3	2.791-11	4.225-11	1.514+00
H2CO3	5.763-06	8.724-06	1.514+00
CA++	5.665-02	1.841-03	3.251-01
CAOH+	1.402-07	1.599-07	1.140+00
CASO3	1.875-04	2.839-04	1.514+00
CACO3	2.518-06	3.812-06	1.514+00
CAHCO3+	9.006-06	1.027-05	1.140+00
CASO4	6.274-03	9.497-03	1.514+00
CANO3+	7.427-04	8.466-04	1.140+00
CACO3(S)	5.873-01	5.873-01	1.000+00
CASO4(S)	2.391+00	2.391+00	1.000+00
CASO3(S)	6.627+00	6.627+00	1.000+00
CA(OH)2(S)	1.216-37	1.216-37	1.000+00
MG++	5.749-01	9.709-01	1.689+00
MGOH+	1.330-03	1.585-03	1.140+00
MGSO3	3.157-02	4.779-02	1.514+00
MGHCO3+	2.281-03	2.601-03	1.140+00
MGSO4	3.879+00	5.871+00	1.514+00
MGCO3	2.128-03	3.221-03	1.514+00
MG(OH)2(S)	5.133+00	5.133+00	1.000+00
MGCO3(S)	1.216-37	1.216-37	1.000+00
NA+	2.595-01	2.042-01	7.870-01
NAOH	1.131-07	1.712-07	1.514+00
NACO3-	3.904-06	4.450-06	1.140+00

50°C
130% theo. LS
50 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
Fly ash and soluble
Na and Cl included

PS#6-FB (continued)

NAHCO3	1.943-05	2.941-05	1.514+00
NAS04-	1.980-02	2.258-02	1.140+00
NANO3	5.695-03	9.621-03	1.514+00
CL-	1.916-01	1.039-01	5.427-01

PS02 =7.87194-11 ATM.
PC02 =4.67309-04 ATM.

PH = 7.755 IONIC STRENGTH = 2.36934+00 RES. E.N. = -4.495-10

PROTOTYPE SIMULATION PS#6-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=4.27836+00	NO3-	=4.93137-01	CA++	=3.51006-02	MG++	=4.49094+00
NA+	=2.84276-01	CL-	=1.91132-01				
SO2	=6.31919-02						
PCO2	=1.43188-01 ATM.						

SCRUBBER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	1.663-05	3.390-05	2.039+00
OH-	1.412-09	1.615-09	1.144+00
HSO3-	3.110-02	3.558-02	1.144+00
SO3--	2.610-05	4.473-05	1.714+00
SO4--	3.546-01	1.773-02	4.999-02
HCO3-	3.556-05	4.069-05	1.144+00
CO3--	4.721-11	8.089-11	1.714+00
NO3-	4.867-01	1.056-01	2.169-01
HSO4-	1.085-04	1.242-04	1.144+00
H2SO3	1.016-04	1.541-04	1.517+00
H2CO3	1.762-03	2.673-03	1.517+00
CA++	5.795-03	1.892-03	3.264-01
CAOH+	7.443-11	8.516-11	1.144+00
CASO3	1.885-04	2.859-04	1.517+00
CACO3	2.127-10	3.226-10	1.517+00
CAHCO3+	1.465-06	1.676-06	1.144+00
CASO4	6.261-03	9.497-03	1.517+00
CANO3+	7.569-04	8.659-04	1.144+00
CACO3(S)	1.217-37	1.217-37	1.000+00
CASO4(S)	2.210-02	2.210-02	1.000+00
CASO3(S)	3.667-37	3.667-37	1.000+00
CA(OH)2(S)	1.216-37	1.216-37	1.000+00
MG++	5.928-01	9.988-01	1.714+00
MGOH+	7.387-07	8.452-07	1.144+00
MGSO3	3.177-02	4.820-02	1.517+00
MGHCO3+	3.715-04	4.250-04	1.144+00
MGSO4	3.876+00	5.879+00	1.517+00
MGCO3	1.900-07	2.730-07	1.517+00
MG(OH)2(S)	1.217-37	1.217-37	1.000+00
MGCO3(S)	1.217-37	1.217-37	1.000+00
NA+	2.594-01	2.044-01	7.878-01
NAOH	5.857-11	8.884-11	1.517+00
NACO3-	3.207-10	3.669-10	1.144+00

50°C
130% theo. LS
50 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
Fly ash and soluble Na and Cl included
10 gpm/ft²
3.94 gpm/ft³
15% LS dissolves in S

PS#6-SB (continued)

NAHCO3	3.083-06	4.876-06	1.517+00
NAS04-	1.922-02	2.199-07	1.144+00
NAN03	5.662-03	8.599-03	1.517+00
CL-	1.911-01	1.025-01	5.364-01

PS02 =2.87040-04 ATM.
C02 =2.17408-03

PH = 4.470 IONIC STRENGTH = 2.38076+00 RES. E.N. = -5.759-10

KP&L SIMULATION KPL#7B-SL

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--=2.70000-02	NO3- =2.00000-03	CA++ =4.05000-02	MG++ =4.50000-03
NA+ =8.00000-04	CL- =5.30000-04		
SO2 =2.70000-02			
CO2 =4.00000-03			

SCRUBBER LIQUID

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	9.558-05	7.944-05	8.311-01
OH-	8.834-10	6.905-10	7.816-01
HSO3-	1.928-02	1.507-02	7.816-01
SO3--	2.285-05	8.526-06	3.732-01
SO4--	1.283-02	4.229-03	3.296-01
HCO3-	3.340-05	2.611-05	7.816-01
CO3--	5.937-11	2.216-11	3.732-01
NO3-	1.938-03	1.406-03	7.256-01
HSO4-	8.884-05	6.944-05	7.816-01
H2SO3	1.549-04	1.572-04	1.015+00
H2CO3	3.960-03	4.019-03	1.015+00
CA++	2.063-02	7.929-03	3.844-01
CAOH+	1.953-10	1.526-10	7.816-01
CASO3	6.662-05	6.761-05	1.015+00
CACO3	3.651-10	3.705-10	1.015+00
CAHCO3+	5.767-06	4.508-06	7.816-01
CASO4	8.355-03	8.479-03	1.015+00
CANO3+	6.190-05	4.838-05	7.816-01
CACO3(S)	3.891-16	3.891-16	1.000+00
CASO4(S)	3.901-03	3.901-03	1.000+00
CASO3(S)	7.480-03	7.480-03	1.000+00
CA(OH)2(S)	2.695-20	2.695-20	1.000+00
MG++	2.694-03	1.006-03	3.732-01
MGOH+	4.656-10	3.639-10	7.816-01
MGSO3	8.449-07	8.574-07	1.015+00
MGHCO3+	3.514-07	2.746-07	7.816-01
MGSO4	1.805-03	1.831-03	1.015+00
MGCO3	7.421-11	7.531-11	1.015+00
MG(OH)2(S)	2.544-22	2.544-22	1.000+00
MGCO3(S)	7.495-21	7.495-21	1.000+00
NA+	7.793-04	6.186-04	7.938-01
NAOH	1.133-13	1.150-13	1.015+00
NACO3-	3.893-13	3.043-13	7.816-01

50°C
75% theo. LS
90% SO_2 Removal
50% SO_2 Oxidation
10 gpm/ft² SL
Est. Soluble Na and Cl

KPL#7B-SL (continued)

NAHCO3	2.830-08	2.872-08	1.015+00
NASO4-	2.032-05	1.588-05	7.816-01
NANO3	3.412-07	3.463-07	1.015+00
CL-	5.300-04	4.094-04	7.725-01

PSO2 =2.93192-04 ATM.
PCO2 =2.15403-01 ATM.

PH = 4.100 IONIC STRENGTH = 8.37738-02 RES. E.N. = -6.187-10

KP&L SIMULATION KPL#7B-SF

INPUT CONCENTRATIONS (MOLES/LITER)

S04--=1.00000E-03 NA+ =1.03200-01 S02 =1.00800-02 C02 =2.24000-03
NA+ =7.47000-04 CL- =8.32000-02 CA++ =5.34000-03 MG++ =5.61000-03

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SCRUBBER FEED

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	2.437-12	2.034-12	8.347-01
OH-	3.414-02	2.696-02	7.898-01
HS03-	4.954-10	3.913-10	7.898-01
S03--	2.222-05	8.648-06	3.891-01
S04--	5.383-03	2.089-03	3.491-01
HC03-	8.877-09	6.972-09	7.898-01
C03--	5.337-07	2.310-07	3.891-01
N03-	7.238-04	5.355-04	7.399-01
HS04-	1.112-12	8.784-13	7.898-01
H2S03	1.032-19	1.046-19	1.013+00
H2C03	2.713-14	2.748-14	1.013+00
CA++	1.951-02	7.818-03	4.007-01
CAOH+	7.439-03	5.876-03	7.898-01
CAS03	6.675-05	6.761-05	1.013+00
CAC03	3.761-06	3.809-06	1.013+00
CAHC03+	1.503-03	1.187-09	7.898-01
CAS04	4.077-03	4.129-03	1.013+00
CANO3+	2.770-05	1.817-05	7.898-01
CAC03(S)	2.236-03	2.236-03	1.000+00
CAS04(S)	6.735-06	6.735-06	1.000+00
CAS03(S)	9.991-03	9.991-03	1.000+00
CA(OH)2(S)	7.044-03	7.044-03	1.000+00
MG++	2.337-08	1.166-08	3.891-01
MGOH+	2.087-07	1.648-07	7.898-01
MGS03	9.960-12	1.003-11	1.013+00
MGHC03+	1.077-15	8.507-16	7.898-01
MGS04	1.036-08	1.049-08	1.013+00
MGC03	8.994-12	9.110-12	1.013+00
MG(OH)2(S)	5.610-03	5.610-03	1.000+00
MGC03(S)	5.077-16	5.077-16	1.000+00
NA+	1.052-03	8.512-04	8.015-01
NAOH	6.019-06	6.178-06	1.013+00
NAC03-	5.528-09	4.366-09	7.898-01

50°C
75% theo. LS
10 mole% MgO in LS
90% SO_2 removal
50% SO_2 oxidation
10 gpm/ft² SL
Est. soluble Na and Cl
30% SO_2, CO_2, and NO_x removal in boiler

KPL#7B-SF (continued)

NAHCO3	1.042-11	1.055-11	1.013+00
NAS04-	1.767-05	1.073-05	7.898-01
NAN03	1.792-07	1.815-07	1.013+00
CL-	6.6[illegible]-04	5.173-04	7.822-01

PS02 =1.3[illegible]C-13 ATM.
PC02 =1.47292-12 ATM.

PH = 11.692 IONIC STRENGTH = 7.30715-02 RES. E.N. = -1.294-09

NAPCA VENTURI SIMULATION NV#2-FB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=5.35914+00	NO3-	=0.00000	CA++ =1.68221+01	MG++ =0.00000
NA+	=0.00000	CL-	=0.00000		
SO2	=5.35914+00				
CO2	=6.74251-02				

FILTER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT	
H+	2.624-12	2.175-12	8.289-01	
OH-	3.245-02	2.518-02	7.761-01	
HSO3-	4.958-10	3.848-10	7.761-01	
SO3--	2.078-05	7.540-06	3.628-01	50°C
SO4--	1.182-02	3.740-03	3.165-01	110% theo. LS
HCO3-	8.383-09	6.506-09	7.761-01	0 mole% MgO
CO3--	5.558-07	2.016-07	3.628-01	70% SO_2 removal
HSO4-	2.165-12	1.680-12	7.761-01	50% SO_2 oxidation
H2SO3	1.052-19	1.069-19	1.016+00	No fly ash, soluble
H2CO3	2.698-14	2.742-14	1.016+00	Na and Cl, and NO_x
CA++	2.401-02	8.967-03	3.735-01	0.50 lbs. liquid H_2O/lb.
CAOH+	8.109-03	6.293-03	7.761-01	non-H_2O in CB
CASO3	6.653-05	6.761-05	1.016+00	
CACO3	3.751-06	3.812-06	1.016+00	
CAHCO3+	1.637-09	1.270-09	7.761-01	
CASO4	9.345-03	9.497-03	1.016+00	
CACO3(S)	6.742-02	6.742-02	1.000+00	
CASO4(S)	5.338+00	5.338+00	1.000+00	
CASO3(S)	5.359+00	5.359+00	1.000+00	
CA(OH)2(S)	6.016+00	6.016+00	1.000+00	

PSO2 =1.99118-19 ATM.

PCO2 =1.46870-12 ATM.

PH = 11.663 IONIC STRENGTH = 9.19569-02 RES. E.N. = -3.067-08

NAPCA VENTURI SIMULATION NV#2-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--=3.89514-02 NO3- =0.00000 CA++ =4.77031-02 MG++ =0.00000
NA+ =0.00000 CL- =0.00000
SO2 =1.79533-02
PCO2 =2.31234-02 ATM.

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	1.499-04	1.251-04	8.346-01
OH-	5.545-10	4.377-10	7.894-01
HSO3-	1.768-02	1.396-02	7.894-01
SO3--	1.224-05	4.755-06	3.884-01
SO4--	1.171-02	4.079-03	3.482-01
HCO3-	2.256-06	1.781-06	7.894-01
CO3--	2.470-12	9.594-13	3.884-01
HSO4-	1.335-04	1.054-04	7.894-01
H2SO3	2.202-04	2.230-04	1.013+00
H2CO3	4.262-04	4.317-04	1.013+00
CA++	2.056-02	8.222-03	3.999-01
CAOH+	1.271-10	1.003-10	7.894-01
CASO3	3.859-05	3.909-05	1.013+00
CACO3	1.642-11	1.663-11	1.013+00
CAHCO3+	4.038-07	3.187-07	7.894-01
CASO4	9.375-03	9.497-03	1.013+00
CACO3(S)	1.215-37	1.215-37	1.000+00
CASO4(S)	1.773-02	1.773-02	1.000+00
CASO3(S)	1.137-12	1.137-12	1.000+00
CA(OH)2(S)	1.215-37	1.215-37	1.000+00

PSO2 =4.15508-04 ATM.
CO2 =4.28826-04

50°C
110% Theo. LS
0 mole% MgO
70% SO_2 removal
50% SO_2 oxidation
No fly ash, soluble Na and Cl, and NO_x
10 gpm SF
1008 gpm SR
No LS dissolves in S

PH = 3.903 IONIC STRENGTH = 7.35605-02 RES. E.N. = -4.097-07

NAPCA VENTURI SIMULATION NV#6-FB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4-- = 1.38232+00 NO3- = 1.97475-01 CA++ = 4.44240+00 MG++ = 0.00000
NA+ = 5.19132-02 CL- = 5.04634-02
SO2 = 1.38232+00
CO2 = 2.46848-02

FILTER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	4.156-12	3.566-12	8.580-01
OH-	2.137-02	1.536-02	7.189-01
HSO3-	3.265-10	2.347-10	7.189-01
SO3--	1.050-05	2.805-06	2.670-01
SO4--	9.145-03	1.391-03	1.521-01
HCO3-	5.520-09	3.968-09	7.189-01
CO3--	2.809-07	7.501-08	2.670-01
NO3-	1.821-01	9.669-02	5.309-01
HSO4-	1.426-12	1.025-12	7.189-01
H2SO3	1.000-19	1.069-19	1.069+00
H2CO3	2.566-14	2.742-14	1.069+00
CA++	9.711-02	2.410-02	2.482-01
CAOH+	1.435-02	1.032-02	7.189-01
CASO3	6.327-05	6.761-05	1.069+00
CACO3	3.567-06	3.812-06	1.069+00
CAHCO3+	2.997-09	2.082-09	7.189-01
CASO4	8.887-03	9.497-03	1.069+00
CANO3+	1.405-02	1.011-02	7.189-01
CACO3(S)	2.468-02	2.468-02	1.000+00
CASO4(S)	1.364+00	1.364+00	1.000+00
CASO3(S)	1.382+00	1.382+00	1.000+00
CA(OH)2(S)	1.544+00	1.544+00	1.000+00
NA+	5.00E-02	3.605-02	7.201-01
NAOH	1.395-04	1.490-04	1.069+00
NACO3-	8.348-08	6.001-08	7.189-01
NAHCO3	7.528-11	8.045-11	1.069+00
NASO4-	4.235-04	3.044-04	7.189-01
NANO3	1.299-03	1.398-03	1.069+00
CL-	5.046-02	3.324-02	6.586-01

PSO2 = 1.39118-10 ATM.
PCO2 = 1.46870-12 ATM.

PH = 11.448 IONIC STRENGTH = 3.78944-01 RES. E.N. = -7.948-09

50°C
113.7% theo. LS
0 mole% MgO
70% SO_2 removal
50% SO_2 oxidation
Fly ash, soluble Na and Cl, and NO_x included
1.00 lbs. liquid H_2O/lb non-H_2O in CB

NAPCA VENTURI SIMULATION NV#6-SB

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=4.20566-02	NO3-	=1.97403-01	CA++	=1.55161-01	MG++	=0.00000
NA+	=5.12709-02	CL-	=4.98332-02				
SO2	=2.39990-02						
PCO2	=2.31179-02 ATM.						

SCRUBBER BOTTOMS

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	2.241-04	1.921-04	8.573-01
OH-	3.965-10	2.850-10	7.189-01
HSO3-	1.690-02	1.215-02	7.189-01
SO3--	1.009-05	2.695-06	2.671-01
SO4--	8.745-03	1.337-03	1.529-01
HCO3-	1.613-06	1.159-06	7.189-01
CO3--	1.523-12	4.067-13	2.671-01
NO3-	1.815-01	9.658-02	5.321-01
HSO4-	7.379-05	5.305-05	7.189-01
H2SO3	2.791-04	2.981-04	1.068+00
H2CO3	4.041-04	4.316-04	1.068+00
CA++	1.009-01	2.509-02	2.487-01
CAOH+	2.772-10	1.993-10	7.189-01
CASO3	6.331-05	6.761-05	1.068+00
CACO3	2.014-11	2.151-11	1.068+00
CAHCO3+	8.809-07	6.332-07	7.189-01
CASO4	8.893-03	9.497-03	1.068+00
CANO3+	1.462-02	1.051-02	7.189-01
CACO3(S)	1.216-37	1.216-37	1.000+00
CASO4(S)	2.394-02	2.394-02	1.000+00
CASO3(S)	6.746-03	6.746-03	1.000+00
CA(OH)2(S)	1.216-37	1.216-37	1.000+00
NA+	4.958-02	3.572-02	7.204-01
NAOH	2.586-12	2.748-12	1.068+00
NACO3-	4.484-13	3.224-13	7.189-01
NAHCO3	2.180-08	2.329-08	1.068+00
NASO4-	4.031-04	2.898-04	7.189-01
NANO3	1.286-03	1.373-03	1.068+00
CL-	4.983-02	3.295-02	6.593-01

PSO2 =5.55407-04 ATM.
CO2 =4.06626-04

50°C
113.7% theo. LS
0 mole% MgO
70% SO_2 removed
50% SO_2 oxidation
Fly ash, soluble Na and Cl, and NO_x included
10 gpm SF
2.90 gpm SR
No LS dissolves in S

PH = 3.716 IONIC STRENGTH = 3.75880-01 RES. E.N. = 8.977-10

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APPENDIX C

PRINTOUTS FOR CHEMICAL EQUILIBRIUM COMPUTER PROGRAM VERIFICATION (Section IV-E)

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INPUT CONCENTRATIONS (MOLES/LITER)

SO4--=0.00000 NO3- =0.00000 CA++ =0.00000 MG++ =0.00000
NA+ =0.00000 CL- =0.00000
SO2 =5.61000-01
CO2 =0.00000

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	9.906-02	8.259-02	8.337-01
OH-	1.571-13	1.227-13	7.805-01
HSO3-	9.906-02	7.693-02	7.766-01
SO3--	1.593-07	5.795-08	3.637-01
H2SO3	4.819-01	4.904-01	1.017+00

PSO2 =4.03340-01 ATM.

PH = 1.083 IONIC STRENGTH = 9.90838-0[illegible] RES. E.N. = -3.841-10

C-12

Solubility of SO_2 in water at 25°C - Case 2

INPUT CONCENTRATIONS (MOLES/LITER)

SO4-- =5.07200-01	NO3- =0.00000	CA++ =0.00000	MG++ =0.00000
NA+ =0.00000	CL- =0.00000		
SO2 =1.58000-03			
CO2 =0.00000			

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	5.609-01	5.214-01	9.297-01
OH-	2.631-14	1.943-14	7.384-01
HSO3-	5.429-05	4.194-05	8.523-01
SO3--	2.763-11	5.004-12	1.811-01
SO4--	5.354-02	6.679-03	1.247-01
HSO4-	4.537-01	3.350-01	7.384-01
H2SO3	1.516-03	1.688-03	1.114+00

PSO2 =1.38824-03 ATM.

PH = .283 IONIC STRENGTH = 5.14432-01 RES. E.N. = -2.824-07

NOT REPRODUCIBLE

Solubility of SO_2 in Aqueous H_2SO_4 at 25°C - Case 6

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=0.00000	NO3-	=0.00000	CA++	=3.84000-03	MG++	=0.00000
NA+	=0.00000	CL-	=0.00000				
SO2	=0.00000						
CO2	=1.05000-02						

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRIATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	2.411-07	2.184-07	9.056-01
OH-	1.502-07	1.345-07	8.956-01
HCO3-	7.321-03	6.564-03	8.966-01
CO3--	2.801-06	1.811-06	6.464-01
H2CO3	2.830-03	2.836-03	1.002+00
CA++	3.494-03	2.270-03	6.498-01
CAOH+	8.933-09	8.000-09	8.956-01
CACO3	7.765-06	7.780-06	1.002+00
CAHCO3+	3.383-04	3.029-04	8.956-01

PCO2 =1.20650-01 ATM.

PH = 6.661 IONIC STRENGTH = 1.09240-02 RES. E.N. = 5.485-05

Ca-CO_2-H_2O system at 40°C - Case 5

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=0.00000	NO3-	=0.00000	CA++	=2.42000-01	MG++	=0.00000
NA+	=0.00000	CL-	=0.00000				
SO2	=5.33000-01						
CO2	=0.00000						

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	1.477-03	1.432-03	9.698-01
OH-	5.164-11	3.829-11	7.414-01
HSO3-	4.824-01	3.041-01	6.304-01
SO3--	5.727-05	9.044-06	1.579-01
H2SO3	4.904-02	5.566-02	1.135+00
CA++	2.405-01	5.434-02	2.259-01
CAOH+	7.821-11	5.799-11	7.414-01
CASO3	1.463-03	1.661-03	1.135+00

PSO2 =1.03793-01 ATM.

PH = 2.844 IONIC STRENGTH = 7.23303-01 RES. E.N. = 7.999-06

NOT REPRODUCIBLE

Ca-SO_2-H_2O System at 50°C - Case 1

INPUT CONCENTRATIONS (MOLES/LITER)

SO4-- =8.66600-01	NO3- =0.00000	CA++ =0.00000	MG++ =9.03400-01
NA+ =0.00000	CL- =0.00000		
SO2 =3.43900-01			
CO2 =0.00000			

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	4.281-06	4.825-06	1.127+00
OH-	1.427-08	1.137-08	7.965-01
HSO3-	2.130-01	1.290-01	6.055-01
SO3--	8.473-03	1.139-03	1.344-01
SO4--	1.826-01	1.470-02	8.049-02
HSO4-	1.841-05	1.466-05	7.965-01
H2SO3	6.578-05	7.952-05	1.209+00
MG++	2.976-01	1.198-01	4.025-01
MGOH+	8.960-07	7.137-07	7.965-01
MGSO3	1.218-01	1.473-01	1.209+00
MGSO4	4.839-01	5.850-01	1.209+00

PSO2 =1.48279-04 ATM.

PH = 5.317 IONIC STRENGTH = 1.08401+00 RES. E.N. = -1.642-06

Mg-SO_2-H_2O system at 50°C - Case 7

NOT REPRODUCIBLE

Sea Water Model

INPUT CONCENTRATIONS (MOLES/LITER)

SO4--	=2.84000-02	NO3-	=0.00000	CA++	=1.04000-02	MG++	=5.40000-02
NA+	=4.85200-01	CL-	=5.54000-01				
SO2	=0.00000						
CO2	=2.64000-03						

AQUEOUS SOLUTION EQUILIBRIA

COMPONENT	CONCENTRATION	ACTIVITY	ACTIVITY COEFFICIENT
H+	4.939-09	4.697-09	9.492-01
OH-	2.905-06	2.161-06	7.437-01
SO4--	1.761-02	9.084-03	1.193-01
HCO3-	1.659-03	1.073-03	6.466-01
CO3--	6.129-05	1.071-05	1.748-01
HSO4-	1.264-09	9.397-10	7.437-01
H2CO3	1.004-05	1.130-05	1.125+00
CA++	9.449-03	2.267-03	2.399-01
CAOH+	1.560-07	1.160-07	7.437-01
CACO3	3.427-05	3.855-05	1.125+00
CAHCO3+	5.944-05	4.420-05	7.437-01
CASO4	8.576-04	9.648-04	1.125+00
MG++	4.957-02	1.490-02	3.059-01
MGOH+	1.660-05	1.235-05	7.437-01
MGHCO3+	1.343-04	1.449-04	7.437-01
MGSO4	4.860-03	5.467-03	1.125+00
MGCO3	3.539-04	3.979-04	1.125+00
NA+	4.799-01	3.443-01	7.176-01
NAOH	1.781-07	2.003-07	1.125+00
NACO3-	9.136-05	6.791-05	7.437-01
NAHCO3	1.847-04	2.077-04	1.125+00
NASO4-	5.072-03	3.772-03	7.437-01
CL-	5.540-01	3.462-01	6.246-01

PCO2 =3.30125-04 ATM.

PH = 8.223 IONIC STRENGTH = .71851-01 PES. E.N. = -1.190-07

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APPENDIX D

PROGRAM OPERATING INSTRUCTIONS AND LISTINGS

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PROGRAM NAME: SOLNEQ
PURPOSE: Solves Equilibrium Equations for Aqueous Solutions
PROJECT: 200-002, HEW/NAPCA
DATE: October, 1969

PROGRAM DEFINITION

This routine solves a set of equilibrium equations for aqueous solutions. The equations solved are taken from the following set:

$$K_w = a_{H^+} a_{OH^-} \quad (1)$$

$$K_2 a_{H_2SO_3} = a_{H^+} a_{HSO_3^-} \quad (2)$$

$$K_3 a_{HSO_3^-} = a_{H^+} a_{SO_3^=} \quad (3)$$

$$K_4 a_{HSO_4^-} = a_{H^+} a_{SO_4^=} \quad (4)$$

$$K_5 a_{H_2CO_3} = a_{H^+} a_{HCO_3^-} \quad (5)$$

$$K_6 a_{HCO_3^-} = a_{H^+} a_{CO_3^=} \quad (6)$$

$$K_7 a_{CaOH^+} = a_{Ca^{++}} a_{OH^-} \quad (7)$$

$$K_8 a_{CaSO_3} = a_{Ca^{++}} a_{SO_3^=} \quad (8)$$

$$K_9 a_{CaCO_3} = a_{Ca^{++}} a_{CO_3^=} \quad (9)$$

$$K_{10} a_{CaHCO_3^+} = a_{Ca^{++}} a_{HCO_3^-} \quad (10)$$

$$K_{11} a_{CaSO_4} = a_{Ca^{++}} a_{SO_4^=} \quad (11)$$

$$K_{12} a_{CaNO_3^+} = a_{Ca^{++}} a_{NO_3^-} \quad (12)$$

$$K_{sp}[CaCO_3(S)] \geq a_{Ca^{++}} a_{CO_3^=} \quad (13)$$

$$K_{sp}[CaSO_4(S)] \geq a_{Ca^{++}} a_{SO_4^{=}} \quad (14)$$

$$K_{sp}[CaSO_3(S)] \geq a_{Ca^{++}} a_{SO_3^{=}} \quad (15)$$

$$K_{sp}[Ca(OH)_2(S)] \geq a_{Ca^{++}} a^2_{OH^-} \quad (16)$$

$$K_{17} a_{MgOH^+} = a_{Mg^{++}} a_{OH^-} \quad (17)$$

$$K_{18} a_{MgSO_3} = a_{Mg^{++}} a_{SO_3^{=}} \quad (18)$$

$$K_{19} a_{MgHCO_3^+} = a_{Mg^{++}} a_{HCO_3^-} \quad (19)$$

$$K_{20} a_{MgSO_4} = a_{Mg^{++}} a_{SO_4^{=}} \quad (20)$$

$$K_{21} a_{MgCO_3} = a_{Mg^{++}} a_{CO_3^{=}} \quad (21)$$

$$K_{sp}[Mg(OH)_2(S)] \geq a_{Mg^{++}} a^2_{OH^-} \quad (22)$$

$$K_{sp}[MgCO_3(S)] \geq a_{Mg^{++}} a_{CO_3^{=}} \quad (23)$$

$$K_{24} a_{NaOH} = a_{Na^+} a_{OH^-} \quad (24)$$

$$K_{25} a_{NaCO_3^-} = a_{Na^+} a_{CO_3^{=}} \quad (25)$$

$$K_{26} a_{NaHCO_3} = a_{Na^+} a_{HCO_3^-} \quad (26)$$

$$K_{27} a_{NaSO_4^-} = a_{Na^+} a_{SO_4^{=}} \quad (27)$$

$$K_{28} a_{NaNO_3} = a_{Na^+} a_{NO_3^-} \quad (28)$$

Where: $a_x = \gamma_x M_x$ activity of component x

γ_x = activity coefficient of component x

M_x = molarity (moles/liter) of component x

Also the material balances are included:

$$\text{Total}_{SO_2} = M_{HSO_3^-} + M_{SO_3^=} + M_{H_2SO_3} + M_{CaSO_3} + M_{CaSO_3(S)} + M_{MgSO_3} \quad (29)$$

$$\text{Total}_{CO_2} = M_{HCO_3^-} + M_{CO_3^=} + M_{H_2CO_3} + M_{CaCO_3} + M_{CaHCO_3^+} + M_{CaCO_3(S)} + M_{MgHCO_3^+} + M_{MgCO_3} + M_{MgCO_3(S)} + M_{NaCO_3^-} + M_{NaHCO_3} \quad (30)$$

$$\text{Total}_{SO_4^=} = M_{SO_4^=} + M_{HSO_4^-} + M_{CaSO_4} + M_{CaSO_4(S)} + M_{MgSO_4} + M_{NaSO_4^-} \quad (31)$$

$$\text{total}_{NO_3^-} = M_{NO_3^-} + M_{CaNO_3^+} + M_{NaNO_3} \quad (32)$$

$$\text{Total}_{Ca^{++}} = M_{Ca^{++}} + M_{CaOH^+} + M_{CaSO_3} + M_{CaCO_3} + M_{CaHCO_3^+} + M_{CaSO_4} + M_{CaNO_3^+} + M_{CaCO_3(S)} + M_{CaSO_4(S)} + M_{CaSO_3(S)} + M_{Ca(OH)_2(S)} \quad (33)$$

$$\text{Total}_{Mg^{++}} = M_{Mg^{++}} + M_{MgOH^+} + M_{MgSO_3} + M_{MgHCO_3^+} + M_{MgSO_4} + M_{MgCO_3} + M_{Mg(OH)_2(S)} + M_{MgCO_3(S)} \quad (34)$$

$$\text{Total}_{Na^+} = M_{Na^+} + M_{NaOH} + M_{NaCO_3^-} + M_{NaHCO_3} + M_{NaSO_4^-} + M_{NaNO_3} \quad (35)$$

And finally the electroneutrality equation:

$$M_{H^+} + 2M_{Ca^{++}} + M_{CaOH^+} + M_{CaHCO_3^+} + M_{CaNO_3^+} + 2M_{Mg^{++}} + M_{MgHCO_3^+} + M_{Na^+} - M_{OH^-} - M_{HSO_3^-} - 2M_{SO_3^=} - 2M_{SO_4^=} - M_{HCO_3^-} - 2M_{CO_3^=} - M_{NO_3^-} - M_{HSO_4^-} - M_{NaCO_3^-} - M_{NaSO_4^-} - M_{Cl^-} = 0 \quad (36)$$

The above is the total set of thirty-six equations and thirty-six unknowns. The cloride ion is treated as a constant. Depending upon the input concentration values, the left side of Equations 29-35 and M_{Cl^-}, a condensed set of equations are solved by this routine. For example, if $\text{Total}_{NO_3^-} = 0$, then the variables $M_{NO_3^-}$, $M_{CaNO_3^+}$, and M_{NaNO_3} are eliminated as well as Equations 12, 28, and 32. If all the input concentrations are zero, then the trivial case involving M_{H^+} and M_{OH^-} is solved. Equations 13-16, 22 and 23 are inequalities. They account for the precipitation or dissolution of the solid species. An option is provided for elimination of these species from the set of equations. In addition, the routine has provisions for solving the set of equations when either the partial pressures of SO_2 or CO_2 are input. In this case Equation 2 would become:

$$K_2 p_{SO_2} K_{pSO_2} = a_{H^+} a_{HSO_3^-} \quad (2)'$$

or Equation 5 would be

$$K_5 P_{CO_2} K_{pCO_2} = a_{H^+} a_{HCO_3^-} \qquad (5)'$$

where:

$$M_{H_2SO_3} = P_{SO_2} K_{pSO_2} / \gamma_{H_2SO_3}$$

or,

$$M_{H_2CO_3} = P_{CO_3} K_{pCO_3} / \gamma_{H_2CO_3}$$

with:

P_x = partial pressure of x

K_{px} = partial pressure constant of x

For those cases where a partial pressure is input, total SO_2 or CO_2 becomes a variable.

The equilibrium, solubility, and partial pressure constants are computed for each new input temperature.

PROCESSING METHOD

The set of nonlinear equations are solved by using the Radian library program NOLIN. The variables transferred to this routine are defined by

$$\psi_i = \ell n\ M_i$$

which is the logarithm of the molarities. The equilibrium equations are in the form

$$\ell n\ a_i + \ell n\ a_j - \ell n\ K - \ell n\ a_k = 0$$

and the material balances are written

$$\ell n\left(\text{Total}_x\right) - \ell n\left(\sum M_i\right) = 0$$

The electroneutrality is written

$$\ell n\left(\sum |z_i| M_{i\ \text{pos.}}\right) - \ell n\left(\sum |z_i| M_{i\ \text{neg.}}\right) = 0$$

OPERATING INSTRUCTIONS

A. Calling Sequence:

CALL SOLNEQ (X, NS, CM, PP, TK, IOPT)

B. Arguments:

X = An array containing the initial guesses for the molarities, when the routine returns, X contains the solution.

NS = 1, No solids are considered in the solution.
= 0, Solids are computed.

CM = An array containing the input concentration.
CM(1) = SO_2 (moles/liter)
CM(2) = CO_2
CM(3) = $SO_4^=$
CM(4) = NO_3^-
CM(5) = Ca^{++}
CM(6) = Mg^{++}
CM(7) = Na^+
CM(8) = Cl^-

if CM(I) = 0, then variables and equations involving this species are deleted from the solutions.

PP = An array containing input partial pressure
PP(1) = PSO_2 (atm)
PP(2) = PCO_2
TK = Temperature (Kelvin)
IOPT = 0 Use CM(1) and CM(2) as inputs, compute PP(1) and PP(2).
= 1 Use PP(1) and CM(2) as inputs, compute CM(1) and PP(2).
= 2 Use CM(1) and PP(2) as inputs, compute PP(1) and CM(2).
= 3 Use PP(1) and PP(2) as inputs, compute CM(1) and CM(2).

C. Diagnostic Messages and Error Stops:

If the number of equations does not match the number of variables, the routine exits via CALL EXIT.

D. External References:

There are two routines subordinated to SOLNEQ:

CTEMP
NOLIN

```
@I FOR SOLNEQ
      SUBROUTINE SOLNEQ(X,NS,CM,PP,TK,IOPT)
      COMMON /LIMS/NF,NT
      COMMON/TEMPER/AC,BC,CPK(2)
      COMMON /ACOEF/GLN(50),DGLN(50),IZ(50),FI
      COMMON/FUNC/F(50),CK(50),CT(10)
      COMMON /PPRESS/PK(2),L1,L2
      COMMON /NEW/ IV(36),IE(36),CL
      EXTERNAL EQS,PARTL
      DOUBLE PRECISION F,CK,CT,XLN
      DIMENSION X(1),CM(10),LB(100),PP(2),XLN(37)
C
      DATA ICME1/037677755767 4/ICMV1/037773576737 1/ICME2/037562537 3147/
     1ICMV2/031527731671 7/ICME3/037357676677 3/ICMV3/027757667756 7/ICME4/
     2036737777577 7/ICMV4/017777757767 7/ICME5/035777700037/ICMV5/037777
     300017777/ICME6/033776007777 7/ICMV6/037400777777 7/ICME7/027701777777
     47/ICMV7/000377777777 7/
      DATA (LB(I),I=1,74)/'H+      ',' OH-     ',' HSO3-   ',
     1     'SO3--   ',' HSO4-   ',' SO4--   ',' HCO3-   ',' CO3
     2--   ',' NO3-    ',' H2SO3   ',' H2CO3   ',
     3                  'CA++    ',' CAOH+   ',
     8                                                    '
     4CASO3   ',' CAHSO3+ ',' CASO4   ',' CACO3   ',' CAHCO3+ ',
     5   'CANO3+  ',' CASO4(S)',' CACO3(S)',' CA(OH)2(S)',
     C                  'MG++    ',' MGOH+   ',
     6           ',' MGSO3   ',' MGHSO3+ ',' MGSO4   ',' MGCO3   ',
     7' MG(OH)2(S)',' MGCO3(S)',
     D            'NA+     ',' NAOH    ',' NACO3-  ',
     8   ',' NAHCO3  ',' NASO4-  ',' NANO3   ',' CL-
     9',' */
C
      DEFINE  G(I)=EXP(GLN(I))
C
  100 FORMAT(1H1)
  101 FORMAT(38X,  'AQUEOUS SOLUTION EQUILIBRIA '/)
  102 FORMAT(15X,  'COMPONENT      CONCENTRATION       ACTIVITY
     1          ,  'ACTIVITY COEFFICIENT')
  103 FORMAT(15X,A6,A4,1PE15.3,4X,1PE15.3,1PE18.3)
  104 FORMAT(1X,/15X,'  PH = ',F10.3,10X,'IONIC STRENGTH = ',1PE10.5,
     110X,' RES. E.N. = ',1PE10.3)
  105 FORMAT(32X,  'INPUT CONCENTRATIONS (MOLES/LITER)     '/)
```

```
  106 FORMAT(4X,'SO4-- =',1PE10.5,4X,'NO3- =',1PE10.5,4X,'CA++ =',1PE10.5
     1,4X,                    'MG++ =',1PE10.5/4X,'NA+  =',1PE10.5,4X,
     2                    'CL-  =',1PE10.5)
  111 FORMAT(4X,'SO2  =',1PE10.5)
  112 FORMAT(4X,'CO2  =',1PE10.5)
  113 FORMAT(4X,'PSO2 =',1PE10.5,2X,'ATM.')
  114 FORMAT(4X,'PCO2 =',1PE10.5,2X,'ATM.')
  200 FORMAT(1X,'NO. FUNCTIONS ',I5,10X,'NO. VARIABLES ',I5)
C ***************************************
C *    INITIALIZATION OF ROUTINE        *
C ***************************************
      EPS=1.E-4
      L1=AND(IOPT,1)
      L2=AND(IOPT,2)
      IF(NS.EQ.0) GO TO 20
      IEQ=377763703777B
      IVN=3747703777776
      GO TO 21
   20 CONTINUE
      IEQ=377777777777B
      IVN=377777777777B
   21 CONTINUE
      CL=CM(8)
C ***************************************************************
C *       DETERMINE  WHICH FUNCTIONS AND VARIABLES ARE NEEDED   *
C ***************************************************************
C
      IF(CM(1).NE.0.0.OR .PP(1).NE.0.0)  GO TO 51
      IEQ=AND(IEQ,ICME1)
      IVN=AND(IVN,ICMV1)
   51 IF(CM(2).NE.0.0.OR .PP(2).NE.0.0)  GO TO 52
      IEQ=AND(IEQ,ICME2)
      IVN=AND(IVN,ICMV2)
   52 IF(CM(3).NE.0.) GO TO 53
      IEQ=AND(IEQ,ICME3)
      IVN=AND(IVN,ICMV3)
   53 IF(CM(4).NE.0.) GO TO 54
      IEQ=AND(IEQ,ICME4)
      IVN=AND(IVN,ICMV4)
   54 IF(CM(5).NE.0.) GO TO 55
      IEQ=AND(IEQ,ICME5)
      IVN=AND(IVN,ICMV5)
   55 IF(CM(6).NE.0.) GO TO 56
```

```
      IEQ=AND(IEQ,ICME6)
      IVN=AND(IVN,ICMV6)
   56 IF(CM(7).NE.0.) GO TO 57
      IEQ=AND(IEQ,ICME7)
      IVN=AND(IVN,ICMV7)
   57 IF(CM(8).NE.0.) GO TO 58
      CL=1.E-36
   58 CONTINUE
C
      DO 6 I=3,7
      IF(CM(I).NE.0.) CT(I)=LOG(CM(I))
    6 CONTINJE
      NF=1
      NV=1
      ICK=1
      DO 59 I=2,36
   45 ICE=AND(ICK,IEQ)
      IF(ICE.EQ.0) GO TO 60
      NF=NF+1
      IE(NF)=I
   60 ICV=AND(ICK,IVN)
      IF(ICV.EQ.0) GO TO 59
      NV=NV+1
      IV(NV)=I
   59 ICK=2*ICK
      IF(NF.EQ.NV) GO TO 61
      WRITE(6,200) NF,NV
      CALL EXIT
   61 IE(1)=1
      IV(1)=1
C
C ***********************************************
C *     COMPJTE TEMPERATJRE DEPENDENT VARIABLES  *
C ***********************************************
C
      CALL CTEMP(TK)
C
      WRITE(6,100)
      WRITE(6,105)
      WRITE(6,106) (CM(I),I=3,8)
      IF(LI.EQ.1) GO TO 8
      WRITE(6,111) CM(1)
      IF(CM(1).NE.0.) CT(1)=LOG(CM(1))
```

```
      GO TO 9
    8 WRITE(6,113) PP(1)
      X(10)=PP(1)*CPK(1) +X(3)+X(4)+X(14)+X(21)+X(25)
      PK(1)=LOG(PP(1)*CPK(1))
    9 IF(L2.EQ.2) GO TO 10
      WRITE(6,112) CM(2)
      IF(CM(2).NE.0.) CT(2)=LOG(CM(2))
      GO TO 11
   10 WRITE(6,114) PP(2)
      X(11)=PP(2)*CPK(2) +X(6)+X(7)+X(15)+X(16)+X(19)+X(26)+X(28)+X(30)
     1+X(33)+X(34)
      PK(2)=LOG(PP(2)*CPK(2))
   11 CONTINUE
C
      DO 1 I=1,NF
      NV=IV(I)
      XLN(I)=LOG(X(NV))
    1 CONTINUE
C
      CALL NOLIN(XLN,NF,EPS,EQS,PARTL)
C
      DO 2 I=1,NF
      NV=IV(I)
      X(NV)=EXP(XLN(I))
    2 CONTINUE
C
      IF(L1.EQ.1) CM(1)=X(10)
      IF(L2.EQ.2) CM(2)=X(11)
      IF(L1.EQ.1) X(10)=PP(1)*CPK(1)/G(10)
      IF(L2.EQ.2) X(11)=PP(2)*CPK(2)/G(11)
C
      IS=1
      WRITE(6,101)
      WRITE(6,102)
      DO 3 I=1,NF
      NV=IV(I)
      PG=G(NV)
      A=X(NV)*PG
      IS=2*NV-1
      WRITE(6,103) LB(IS),LB(IS+1),X(NV),A,PG
    3 CONTINUE
      IF(CM(8).EQ.0.) GO TO 4
      PG=G(37)
```

```
      A=CL*PG
      IS=73
      WRITE(6,103) LB(IS),LB(IS+1),CL,A,PG
    4 CONTINUE
C
      IF(L1.EQ.1) GO TO 12
      IF(CM(1).EQ.0.) GO TO 13
      PP(1)=X(10)*G(10)/CPK(1)
      WRITE(6,113) PP(1)
      GO TO 13
   12 WRITE(6,111) CM(1)
   13 IF(L2.EQ.2) GO TO 14
      IF(CM(2).EQ.0.) GO TO 15
      PP(2)=X(11)*G(11)/CPK(2)
      WRITE(6,114) PP(2)
      GO TO 15
   14 WRITE(6,112) CM(2)
   15 CONTINUE
C
      PH=-ALOG10(X(1)*G(1))
      REN=F(NF)
      WRITE(6,104) PH,FI,REN
C
C
      END
```

```
@I FOR PARTL
C
C
C ***************************************************************
C *     THE PARTIAL DERIVATIVES @F/@X ARE PLACED HERE           *
C *     PD(I,J) = -@F(I)/@X(J)                                  *
C ***************************************************************
      SUBROUTINE PARTL(W)
      COMMON/FUNC/F(50),CK(50),CT(10)
      COMMON /GRAD/PD(50,50),AS(50,50),SQ(50)/RESID/GS(50)
      COMMON /ACOEF/GLN(50),DGLN(50),IZ(50)
      COMMON /LIMS/NF,NT
      COMMON /PPRESS/PK(2),L1,L2
      COMMON /NEW/IV(36),IE(36),CL,TH(6)
      DIMENSION W(1),X(50),GD(36,36)
      DOUBLE PRECISION BR
      DOUBLE PRECISION F,CK,CT,W,X,GD
      DOUBLE PRECISION PD,AS,SQ,GS
C
      DEFINE Y(I)=EXP(X(I))
C
C ***************************************************************
C         ZERO UNUSED MOLARITIES AND CONVERT                    *
C ***************************************************************
      DO 5 I=1,36
      DO 6 J=1,36
      GD(I,J)=0.
    6 CONTINUE
    5 CONTINUE
      DO 1 I=1,36
      X(I)=-90.
    1 CONTINUE
C
      DO 2 I=1,NF
      NV=IV(I)
      X(NV)=W(I)
    2 CONTINUE
C
      GD( 1, 1)=-1.0
      GD( 1, 2)=-1.0
      GD( 2, 1)=-1.0
```

```
GD( 2, 3)=-1.0
GD( 2,10)=+1.0
IF(L1.EQ.1) GD(2,10)=0.
GD( 3, 1)=-1.0
GD( 3, 4)=-1.0
GD( 3, 3)=+1.0
GD( 4, 1)=-1.0
GD( 4, 5)=-1.0
GD( 4, 9)=+1.0
GD( 5, 1)=-1.0
GD( 5, 6)=-1.0
GD( 5,11)=+1.0
IF(L2.EQ.2) GD(5,11)=0.
GD( 6, 1)=-1.0
GD( 6, 7)=-1.0
GD( 6, 6)=+1.0
GD( 7,12)=-1.0
GD( 7, 2)=-1.0
GD( 7,13)=+1.0
GD( 8,12)=-1.0
GD( 8, 4)=-1.0
GD( 8,14)=+1.0
GD( 9,12)=-1.0
GD( 9, 7)=-1.0
GD( 9,15)=+1.0
GD(10,12)=-1.0
GD(10, 6)=-1.0
GD(10,16)=+1.0
GD(11,12)=-1.0
GD(11, 5)=-1.0
GD(11,17)=+1.0
GD(12,12)=-1.0
GD(12, 8)=-1.0
GD(12,18)=+1.0
GD(13, 7)=-1.0
GD(13,12)=-1.0
GD(13,19)=1.
GD(14, 5)=-1.0
GD(14,12)=-1.0
GD(14,20)=1.
GD(15, 4)=-1.0
GD(15,12)=-1.0
GD(15,21)=1.
```

```
      GD(16, 2)=-2.0
      GD(16,12)=-1.0
      GD(16,22)=1.
      GD(17,23)=-1.0
      GD(17, 2)=-1.0
      GD(17,24)=+1.0
      GD(18,23)=-1.0
      GD(18, 4)=-1.0
      GD(18,25)=+1.0
      GD(19,23)=-1.0
      GD(19, 6)=-1.0
      GD(19,26)=+1.0
      GD(20,23)=-1.0
      GD(20, 5)=-1.0
      GD(20,27)=+1.0
      GD(21,23)=-1.0
      GD(21, 7)=-1.0
      GD(21,28)=+1.0
      GD(22,23)=-1.0
      GD(22, 2)=-2.0
      GD(22,29)=1.
      GD(23, 7)=-1.0
      GD(23,23)=-1.0
      GD(23,30)=1.
      GD(24,31)=-1.0
      GD(24, 2)=-1.0
      GD(24,32)=+1.0
      GD(25,31)=-1.0
      GD(25, 7)=-1.0
      GD(25,33)=+1.0
      GD(26,31)=-1.0
      GD(26, 6)=-1.0
      GD(26,34)=+1.0
      GD(27,31)=-1.0
      GD(27, 5)=-1.0
      GD(27,35)=+1.0
      GD(28,31)=-1.0
      GD(28, 8)=-1.0
      GD(28,36)=+1.0
      BR=Y(3)+Y(4)+Y(10)+Y(14)+Y(21)+Y(25)
      IF(L1.EQ.1) BR=BR-Y(10)+EXP(PK(1)-CLN(10))
      GD(29, 3)=Y( 3)/BR
      GD(29, 4)=Y( 4)/BR
```

```
      GD(29,10)=Y(10)/BR
      IF(L1.EQ.1) GD(29,10)=-1.
      GD(29,14)=Y(14)/BR
      GD(29,21)=Y(21)/BR
      GD(29,25)=Y(25)/BR
      BR=Y(6)+Y(7)+Y(11)+Y(15)+Y(16)+Y(19)+Y(26)+Y(28)+Y(30)+Y(33)+Y(34)
      IF(L2.EQ.2) BR=BR-Y(11)+EXP(PK(2)-GLN(11))
      GD(30, 6)=Y( 6)/BR
      GD(30, 7)=Y( 7)/BR
      GD(30,11)=Y(11)/BR
      IF(L2.EQ.2) GD(30,11)=-1.
      GD(30,15)=Y(15)/BR
      GD(30,16)=Y(16)/BR
      GD(30,19)=Y(19)/BR
      GD(30,26)=Y(26)/BR
      GD(30,28)=Y(28)/BR
      GD(30,30)=Y(30)/BR
      GD(30,33)=Y(33)/BR
      GD(30,34)=Y(34)/BR
      BR=Y(5)+Y(9)+Y(17)+Y(20)+Y(27)+Y(35)
      GD(31, 5)=Y( 5)/BR
      GD(31, 9)=Y( 9)/BR
      GD(31,17)=Y(17)/BR
      GD(31,20)=Y(20)/BR
      GD(31,27)=Y(27)/BR
      GD(31,35)=Y(35)/BR
      BR=Y(8)+Y(18)+Y(36)
      GD(32,36)=Y(35)/BR
      GD(32, 8)=Y( 8)/BR
      GD(32,18)=Y(18)/BR
      BR=Y(12)+Y(13)+Y(14)+Y(15)+Y(16)+Y(17)+Y(18)+Y(19)+Y(20)+Y(21)
     1+Y(22)
      GD(33,12)=Y(12)/BR
      GD(33,13)=Y(13)/BR
      GD(33,14)=Y(14)/BR
      GD(33,15)=Y(15)/BR
      GD(33,16)=Y(16)/BR
      GD(33,17)=Y(17)/BR
      GD(33,18)=Y(18)/BR
      GD(33,19)=Y(19)/BR
      GD(33,20)=Y(20)/BR
      GD(33,21)=Y(21)/BR
      GD(33,22)=Y(22)/BR
```

```
      BR=Y(23)+Y(24)+Y(25)+Y(26)+Y(27)+Y(28)+Y(29)+Y(30)
      GD(34,23)=Y(23)/BR
      GD(34,24)=Y(24)/BR
      GD(34,25)=Y(25)/BR
      GD(34,26)=Y(26)/BR
      GD(34,27)=Y(27)/BR
      GD(34,28)=Y(28)/BR
      GD(34,29)=Y(29)/BR
      GD(34,30)=Y(30)/BR
      BR=Y(31)+Y(32)+Y(33)+Y(34)+Y(35)+Y(36)
      GD(35,31)=Y(31)/BR
      GD(35,32)=Y(32)/BR
      GD(35,33)=Y(33)/BR
      GD(35,34)=Y(34)/BR
      GD(35,35)=Y(35)/BR
      GD(35,36)=Y(36)/BR
      BR=Y(1)+2*Y(12)+Y(13)+Y(16)+Y(18)+2*Y(23)+Y(24)+Y(26)+Y(31)
      GD(36, 1)=-  Y( 1)/BR
      GD(36,12)=-2*Y(12)/BR
      GD(36,13)=-  Y(13)/BR
      GD(36,16)=-  Y(16)/BR
      GD(36,18)=-  Y(18)/BR
      GD(36,23)=-2*Y(23)/BR
      GD(36,24)=-  Y(24)/BR
      GD(36,26)=-  Y(26)/BR
      GD(36,31)=-  Y(31)/BR
      BR=Y(2)+Y(3)+2*Y(4)+2*Y(5)+Y(6)+2*Y(7)+Y(8)+Y(9)+Y(33)+Y(35)+CL
      GD(36, 2)=  Y( 2)/BR
      GD(36, 3)=  Y( 3)/BR
      GD(36, 4)=2*Y( 4)/BR
      GD(36, 5)=2*Y( 5)/BR
      GD(36, 6)=  Y( 6)/BR
      GD(36, 7)=2*Y( 7)/BR
      GD(36, 8)=  Y( 8)/BR
      GD(36, 9)=  Y( 9)/BR
      GD(36,33)=  Y(33)/BR
      GD(36,35)=  Y(35)/BR
C
      DO 3 I=1,NF
      NE=IE(I)
      DO 4 J=1,NF
      NV=IV(J)
      PD(I,J)=GD(NE,NV)
```

```
 4  CONTINUE
 3  CONTINUE
    RETURN
    END
```

```
@I FOR GAMMA
      SUBROUTINE GAMMA(X)
C ***************************************************************************
C *    THIS ROUTINE COMPUTES LN(G(I)) AS A FUNCTION OF EXP(X(I))            *
C ***************************************************************************
      COMMON/NEW/IV(36),IE(36),CL
      COMMON /TEMPER/AC,BC
      COMMON /ACOEF/ GLN(50),DGLN(50),IZ(50),FI
      COMMON /LIMS/NF,NT
      DOUBLE PRECISION X
      DIMENSION X(1),A(50),B(50),U(50)
      DATA (IZ(I),I=1,37)/1,1,1,4,4,1,4,1,1,0,0,4,1,0,0,1,0,1,0,0,0,0,4,
     11,0,1,0,0,0,0,1,0,1,0,1,0,1/
      DATA U(10)/.076/U(11)/.076/U(14)/.076/U(15)/.076/U(17)/.076/U(25)/
     1.076/U(27)/.076/U(28)/.076/U(32)/.076/U(34)/.076/U(36)/.076/
      DATA (A(I),I=1,37)   /  6.00000   ,  3.00000   ,  4.50000   ,
     *  4.50000   ,  3.00000   ,  4.50000   ,  4.50000   ,  2.00000   ,
     *  3.00000   ,  3.00000   ,  3.00000   ,  4.50000   ,  3.00000   ,
     *  3.00000   ,  3.00000   ,  3.00000   ,  3.00000   ,  3.00000   ,
     *  3.00000   ,  3.00000   ,  3.00000   ,  3.00000   ,  3.00000   ,
     *  3.00000   ,  3.00000   ,  3.00000   ,  3.00000   ,  3.00000   ,
     *  3.00000   ,  3.00000   ,  5.00000   ,  3.00000   ,  3.00000   ,
     *  3.00000   ,  3.00000   ,  3.00000   ,  4.00000   /
      DATA (B(I),I=1,37)   /  .400000   ,  .300000   ,  .000000   ,
     *  .000000   ,  .000000   ,  .000000   ,  .000000   , -.200000   ,
     *  .300000   ,  .300000   ,  .300000   ,  .100000   ,  .300000   ,
     *  .300000   ,  .300000   ,  .300000   ,  .300000   ,  .300000   ,
     *  .300000   ,  .300000   ,  .300000   ,  .300000   ,  .300000   ,
     *  .300000   ,  .300000   ,  .100000   ,  .300000   ,  .300000   ,
     *  .300000   ,  .300000   ,  .300000   ,  .000000   /
C
      DEFINE Y(I)=EXP(X(I))
C
      FI=0.
      DO 1 I=1,36
      FI=FI+IZ(I)*Y(I)
    1 CONTINUE
      FI=FI+CL
      FI=FI/2.
      SFI=SQRT(FI)
```

```
C
      DO 2 I=1,37
      DNM=1.+BC*A(I)*SFI
      GLN(I)=AC*IZ(I)*(-SFI/DNM+R(I)*FI)+2.3026*U(I)*FI
    2 CONTINUE
      RETURN
      END
```

```
@I FOR DELTA
      SUBROUTINE DELTA(DELT,XL)
C ***************************************************************
C *    THIS ROUTINE FINDS THE CORRECTION VECTOR                 *
C ***************************************************************
      COMMON /GRAD/PD(50,50),AS(50,50),SQ(50)
      COMMON /RESID/ GS(50)
      COMMON /LIMS/NF
      COMMON/FUNC/F(50),CK(50),CT(10)
      DOUBLE PRECISION A,B,DETRM
      DOUBLE PRECISION PD,AS,SQ,GS,DELT
      DIMENSION A(50,50),B(50,1),DELT(1)
C
      DO 1 I=1,50
      B(I,1)=0.
      B(I,1)=GS(I)
      DO 2 J=1,50
      A(I,J)=0.
      A(I,J)=AS(I,J)
    2 CONTINUE
    1 CONTINUE
C
      DO 3 I=1,NF
      A(I,I)=A(I,I)+XL
    3 CONTINUE
C
      CALL MATIN(A,NF,B,1,DETRM)
C
      AMAG=0.
      DO 4 I=1,NF
      DELT(I)=B(I,1)/SQ(I)
      AMAG=AMAG+DELT(I)*DELT(I)
    4 CONTINUE
      AMAG=SQRT(AMAG)
      IF(AMAG.LT.10.) RETURN
      DO 7 I=1,NF
      DELT(I)=10.*DELT(I)/AMAG
    7 CONTINUE
      RETURN
      END
```

```
@I FOR EQS
      SUBROUTINE EQS(W)
C ***************************************************************
C *    N FUNCTIONS OF THE  N-VECTOR X  ARE SUPPLIED HERE        *
C ***************************************************************
      COMMON/FUNC/F(50),CK(50),CT(10)
      COMMON /ACOEF/GLN(50),DGLN(50),IZ(50)
      COMMON /LIMS/NF
      COMMON /PPRESS/PK(2),L1,L2
      COMMON /NEW/ IV(36),IE(36),CL,TH(6)
      DIMENSION W(1),X(37),EQ(37)
      DOUBLE PRECISION F,CK,CT,W,X,EQ,TE
      DOUBLE PRECISION FNEQ
C
      DEFINE Y(I)=EXP(X(I))
C
      DO 3 I=1,36
      X(I)=-85.
    3 CONTINUE
      DO 1 I=1,NF
      NV=IV(I)
      X(NV)=W(I)
    1 CONTINUE
C
      CALL GAMMA(X)
C
      EQ( 1)=GLN( 1)+GLN( 2)+X( 1)+X( 2)-CK( 1)
      IF(L1.EQ.1) GO TO 4
      EQ( 2)=GLN( 1)+GLN( 3)+X( 1)+X( 3)-GLN(10)-X(10)-CK( 2)
      EQ(29)=CT(1)-LOG(Y(3)+Y(4)+Y(10)+Y(14)+Y(21)+Y(25))
      GO TO 5
    4 EQ(2)=GLN(1)+GLN(3)+X(1)+X(3)-PK(1)-CK(2)
      EQ(29)=X(10)  -LOG(Y(3)+Y(4)+Y(14)+Y(21)+Y(25)+EXP(PK(1)-GLN(10)))
    5 CONTINUE
      EQ( 3)=GLN( 1)+GLN( 4)+X( 1)+X( 4)-GLN( 3)-X( 3)-CK( 3)
      EQ( 4)=GLN( 1)+GLN( 5)+X( 1)+X( 5)-GLN( 9)-X( 9)-CK( 4)
      IF(L2.EQ.2) GO TO 6
      EQ( 5)=GLN( 1)+GLN( 6)+X( 1)+X( 6)-GLN(11)-X(11)-CK( 5)
      EQ(30)=CT(2)-LOG(Y(6)+Y(7)+Y(11)+Y(15)+Y(16)+Y(19)+Y(26)+Y(28)
     1+Y(30)+Y(33)+Y(34))
      GO TO 7
```

```
6 EQ(5)=GLN(1)+GLN(6)+X(1)+X(6)-PK(2)-CK(5)
  EQ(30)=X(11)  -LOG(Y(6)+Y(7)+Y(15)+Y(16)+Y(19)+Y(26)+Y(28)+Y(30)
 1+Y(33)+Y(34)+EXP(PK(2)-GLN(11)))
7 CONTINUE
  EQ( 6)=GLN( 1)+GLN( 7)+X( 1)+X( 7)-GLN( 6)-X( 6)-CK( 6)
  EQ( 7)=GLN(12)+GLN( 2)+X(12)+X( 2)-GLN(13)-X(13)-CK( 7)
  EQ( 8)=GLN(12)+GLN( 4)+X(12)+X( 4)-GLN(14)-X(14)-CK( 8)
  EQ( 9)=GLN(12)+GLN( 7)+X(12)+X( 7)-GLN(15)-X(15)-CK( 9)
  EQ(10)=GLN(12)+GLN( 6)+X(12)+X( 6)-GLN(16)-X(16)-CK(10)
  EQ(11)=GLN(12)+GLN( 5)+X(12)+X( 5)-GLN(17)-X(17)-CK(11)
  EQ(12)=GLN(12)+GLN( 8)+X(12)+X( 8)-GLN(18)-X(18)-CK(12)
  EQ(13)=GLN(12)+GLN(7)+X(12)+X(7)-CK(13)
  EQ(13)=FNEQ(EQ(13),X(19))
  EQ(14)=GLN(12)+GLN(5)+X(12)+X(5)-CK(14)
  EQ(14)=FNEQ(EQ(14),X(20))
  EQ(15)=GLN(12)+GLN(4)+X(12)+X(4)-CK(15)
  EQ(15)=FNEQ(EQ(15),X(21))
  EQ(16)=GLN(12)+2*GLN(2)+X(12)+2*X(2)-CK(16)
  EQ(16)=FNEQ(EQ(16),X(22))
  EQ(17)=GLN(23)+GLN( 2)+X(23)+X( 2)-GLN(24)-X(24)-CK(17)
  EQ(18)=GLN(23)+GLN( 4)+X(23)+X( 4)-GLN(25)-X(25)-CK(18)
  EQ(19)=GLN(23)+GLN( 6)+X(23)+X( 6)-GLN(26)-X(26)-CK(19)
  EQ(20)=GLN(23)+GLN( 5)+X(23)+X( 5)-GLN(27)-X(27)-CK(20)
  EQ(21)=GLN(23)+GLN( 7)+X(23)+X( 7)-GLN(28)-X(28)-CK(21)
  EQ(22)=GLN(23)+2*GLN(2)+X(23)+2*X(2)-CK(22)
  EQ(22)=FNEQ(EQ(22),X(29))
  EQ(23)=GLN(23)+GLN(7)+X(23)+X(7)-CK(23)
  EQ(23)=FNEQ(EQ(23),X(30))
  EQ(24)=GLN(31)+GLN( 2)+X(31)+X( 2)-GLN(32)-X(32) CK(24)
  EQ(25)=GLN(31)+GLN( 7)+X(31)+X( 7)-GLN(33)-X(33)-CK(25)
  EQ(26)=GLN(31)+GLN( 6)+X(31)+X( 6)-GLN(34)-X(34)-CK(26)
  EQ(27)=GLN(31)+GLN( 5)+X(31)+X( 5)-GLN(35)-X(35)-CK(27)
  EQ(28)=GLN(31)+GLN( 8)+X(31)+X( 8)-GLN(36)-X(36)-CK(28)
  EQ(31)=CT(3)-LOG(Y(5)+Y(9)+Y(17)+Y(20)+Y(27)+Y(35))
  EQ(32)=CT(4)-LOG(Y(8)+Y(18)+Y(36))
  EQ(33)=CT(5)-LOG(Y(12)+Y(13)+Y(14)+Y(15)+Y(16)+Y(17)+Y(18)+Y(19)
 1+Y(20)+Y(21)+Y(22))
  EQ(34)=CT(6)-LOG(Y(23)+Y(24)+Y(25)+Y(26)+Y(27)+Y(28)+Y(29)+Y(30))
  EQ(35)=CT(7)-LOG(Y(31)+Y(32)+Y(33)+Y(34)+Y(35)+Y(36))
  EQ(36)=LOG(Y(1)+2*Y(12)+Y(13)+Y(16)+Y(18)+2*Y(23)+Y(24)+Y(26)
 1+Y(31))
  EQ(36)=EQ(36)-LOG(Y(2)+Y(3)+2*Y(4)+2*Y(5)+Y(6)+2*Y(7)+Y(8)+Y(9)
 1+Y(33)+Y(35)+CL)
```

```
C
      DO 2 I=1,NF
      NE=IE(I)
      NV=IV(I)
      W(I)=X(NV)
      F(I)=EQ(NE)
    2 CONTINUE
      RETURN
      END
```

```
@I FOR ASTAR
      SUBROUTINE ASTAR(X,PARTL)
C ***************************************************************************
C *    THIS ROUTINE  MULTIPLIES THE DERIVATIVE  MATRIX BY ITS               *
C *    TRANSPOSE AND THEN SCALES THE PRODUCT                                *
C ***************************************************************************
      COMMON /GRAD/PD(50,50),AS(50,50),SQ(50)
      COMMON /LIMS/NF
      DOUBLE PRECISION SUM
      DOUBLE PRECISION PD,AS,SQ,X
      DIMENSION X(1)
C
      CALL PARTL(X)
      DO 1 I=1,NF
      SUM=0.
      DO 2 K=1,NF
      SUM=SUM+PD(K,I)*PD(K,I)
    2 CONTINUE
      SQ(I)=SQRT(SUM)
      AS(I,I)=1.
    1 CONTINUE
C
      NF1=NF-1
      DO 3 I=1,NF1
      JS=I+1
      DO 4 J=JS,NF
      SUM=0.
      DO 5 K=1,NF
      SUM=SUM+PD(K,I)*PD(K,J)
    5 CONTINUE
      AS(I,J)=SUM/(SQ(I)*SQ(J))
      AS(J,I)=AS(I,J)
    4 CONTINUE
    3 CONTINUE
      RETURN
      END
```

```
aI FOR CTEMP
      SUBROUTINE CTEMP(TK)
      COMMON /PPRESS/PK(2),L1,L2
      COMMON/FUNC/F(50),CK(50),CT(10)
      COMMON/TEMPER/AC,BC,CPK(2)
      DIMENSION A(30),B(30),C(30),D(30),LB(60),EK25(30)
      DOUBLE PRECISION F,CK,CT
      DATA (LB(I),I=1,60)/'H2O   ',' ','H2SO3 ',' ','HSO3  ',' '
     1     ,'HSO4  ',' ','H2CO3 ',' ','HCO3  ',' ','CAO
     2H+ ',' ','CASO3 ',' ','CACO3 ',' ','CAHCO3',' '+
     3',','CASO4 ',' ','CANO3+',' ','CAC03(',' ','S)   ',' ','
     4CASO4(',' ','S)   ',' ','CASO3(',' ','S)   ',' ','CA(OH)',' ','2(S)  ',' ','MGOH+ ',' '
     5   ,' ','MGSO3 ',' ','MGHCO3',' ','+   ',' ','MGSO4 ',' ','MGCO3
     6',' ','MG(OH)',' ','2(S)  ',' ','MGCO3(',' ','S)   ',' ','NAOH  ',' ','NAHCO3',' '
     7NACO3-',' ','NASO4-',' ','NANO3 ',' '
     8   ,' ','PP(SO2',' ')   ',' ','PP(CO2',' ')   '/
      DATA (EK25(I),I=1,30)/  .10129E-13,  .12957E-01,  .62207E-07,
     *  .10396E-01,  .44513E-06,  .46817E-10,  .42229E-01,  .39999E-03,
     *  .62996E-03,  .55002E-01,  .48969E-02,  .484850   ,  .48695E-08,
     *  .24000E-04,  .84004E-07,  .93440E-05,  .26001E-02,  .11997E-02,
     *  .110010   ,  .56636E-02,  .39999E-03,  .12552E-10,  .21500E-04,
     *  3.71540   ,  .54002E-01,  1.77830   ,  .190240   ,  2.51190   ,
     *  1.21580   ,  .34215E-01/
      DATA (A(I),I=1,30)   /   4471.0   ,  -843.67   ,  -633.84   ,
     *   475.14   ,  3404.7   ,  2902.4   ,  -273.00   ,  -504.80   ,
     *  -475.48   ,  -301.85   ,  2572.1   ,  -1245.0   ,  -1660.0   ,
     *  4944.0   ,  .00000   ,  530.49   ,  -517.99   ,  -432.50   ,
     *  -235.08   ,  -1057.9   ,  -504.80   ,  -480.85   ,  -955.14   ,
     *  .00000   ,  -303.41   ,  .00000   ,  -241.00   ,  .00000   ,
     *  -1370.0   ,  -1015.0   /
      DATA (B(I),I=1,30)   /   .00000   ,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   ,  .00000   ,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   ,  23.150   ,  .00000   ,  .00000   ,
     *  37.745   ,  .00000   ,  -12.972   ,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   ,  .00000   ,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   ,  .00000   ,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   /
      DATA (C(I),I=1,30)   /   .1706E-01,  .00000   ,  .00000   ,
     *  .18222E-01,  .32786E-01,  .2379E-01,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   ,  .00000   ,  .00000   ,  .00000   ,
     *  .00000   ,  .00000   ,  .32331E-01,  .00000   ,  .00000   ,
```

```
     *    .00000   ,    .00000   ,    .00000   ,    .00000   ,    .00000   ,
     *    .00000   ,    .00000   ,    .00000   ,    .00000   ,    .00000   ,
     *    .00000   ,    .00000   /
      DATA (D(I),I=1,30)   /   6.0875   ,  -4.7171   ,  -9.3320   ,
     *    5.0435   ,   14.843   ,    6.4980   ,   -2.2900   ,   -5.0910   ,
     *   -4.7954   ,   -2.2720   ,    63.600   ,   -4.4900   ,   -13.880   ,
     *    105.36   ,   -7.0757   ,   -25.709   ,   -4.3223   ,   -4.3715   ,
     *   -1.7470   ,   -5.7950   ,   -5.0910   ,   -12.514   ,   -7.8710   ,
     *    .57000   ,   -2.2852   ,    .25000   ,   -1.5290   ,    .40000   ,
     *   -4.5100   ,   -4.8700   /
C
  100 FORMAT(1H1)
  101 FORMAT(9X,A6,A4,6(1PE10.4,5X))
  102 FORMAT(9X,'REACTANT     K(25 C)',8X,'K(TEMP)',10X,'A',14X,'B',14X,
     *'C',14X,'D'/)
  103 FORMAT(44X,  'EQUILIBRIUM CONSTANTS')
  104 FORMAT(//,21X,'THIS PROGRAM DEVELOPED BY RADIAN CORP. UNDER NAPCA/
     *HEW SPONSORSHIP')
  107 FORMAT(35X,  ' TEMPERATURE',F10.3,'   DEGREES C'//)
C
      IF(TOLD.EQ.TK) RETURN
      TC=TK-273.16
      WRITE(6,100)
      WRITE(6,107) TC
      WRITE(6,103)
      WRITE(6,102)
      TC2=TC*TC
      DC=87.740-0.40008*TC+9.398E-4*TC2-1.410E-6*TC2*TC
      AC=1.8246E6/(DC*TK*SQRT(DC*TK))
      AC=2.3026*AC
      BC=50.29/SQRT(DC*TK)
C
      DM=2.3025851
      DO  1  I=1,28
      D(3)=-9.424
      CK(I)=DM*(-A(I)/TK-B(I)*ALOG10(TK)-C(I)*TK+D(I))
      IF(I.EQ.14.AND.TC.GT.40.) CK(14)=DM*(-1200.9/TK+6.6489*ALOG10(TK)
     *-.032057*TK-7.084)
      EK=EXP(CK(I))
      IS=2*I-1
      WRITE(6,101) LB(IS),LB(IS+1),EK25(I),EK,A(I),B(I),C(I),D(I)
    1 CONTINUE
C
```

```
      DO  2 I=29, 30
      TEMP =DM*(-A(I)/TK-B(I)*ALOG10(TK)-C(I)*TK+D(I))
      EK=EXP(TEMP)
      J=I-28
      CPK(J)=EK
      IS=2*I-1
      WRITE(6, 101) LB(IS),LB(IS+1),EK25(I),EK, A(I),B(I), C(I),D(I)
    2 CONTINUE
      WRITE(6, 104)
      TOLD=TK
      RETURN
      END
```

```
@I FOR GSTAR
      SUBROUTINE GSTAR(X,EQS)
C  * ************************************
C  *            *     T                 *
C  *          G (X)=B (X)*F(X)          *
C  * ************************************
      COMMON /RESID/ GS(50)
      COMMON /GRAD/PD(50,50),AS(50,50),SQ(50)
      COMMON/FUNC/F(50),CK(50),CT(10)
      COMMON /LIMS/NF
      DOUBLE PRECISION SUM
      DOUBLE PRECISION PD,AS,SQ,GS
      DOUBLE PRECISION F,CK,CT,X
      DIMENSION X(1)
C
      CALL EQS(X)
C
C       ASSUME THE PARTIALS HAVE BEEN EVALUATED
C
      DO 1 I=1,NF
      SUM=0.
      DO 2 K=1,NF
      SUM=SUM+PD(K,I)*F(K)
    2 CONTINUE
      GS(I)=SUM/SQ(I)
    1 CONTINUE
      RETURN
      END
```

```
aN FOR MATIN
      SUBROUTINE MATIN (A,N,B,M,DETERM)
      DOUBLE PRECISION A,B,DETERM,PIVOT,AMAX,SWAP,T
      DIMENSION IPIVOT(50),A(50,50),B(50, 1),INDEX(50,2),PIVOT(50)
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX, T, SWAP)          F402
C
C     INITIALIZATION
C
   10 DETERM=1.0
   15 DO 20 J=1,N
   20 IPIVOT(J)=0
   30 DO 550 I=1,N
C
C     SEARCH FOR PIVOT ELEMENT
C
   40 AMAX=0.0
   45 DO 105 J=1,N
   50 IF (IPIVOT(J)-1) 60,105,60
   60 DO 100 K=1,N
   70 IF (IPIVOT(K)-1) 80,100,740
   80 IF (ABS(AMAX)-ABS(A(J,K))) 85,100,100
   85 IROW=J
   90 ICOLUM=K
   95 AMAX=A(J,K)
  100 CONTINUE
  105 CONTINUE
  106 IF (ABS(AMAX).LE.0.0) GO TO 739
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
C
C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
  130 IF (IROW-ICOLUM) 140,260,140
  140 DETERM = -DETERM
  150 DO 200 L=1,N
  160 SWAP=A(IROW,L)
  170 A(IROW,L)=A(ICOLUM,L)
  200 A(ICOLUM,L)=SWAP
  205 IF(M)260,260,210
  210 DO 250 L=1,M
  220 SWAP=B(IROW,L)
  230 B(IROW,L)=B(ICOLUM,L)
```

```
  250 B(ICOLUM,L)=SWAP
  260 INDEX(I,1)=IROW
  270 INDEX(I,2)=ICOLUM
  310 PIVOT(I)=A(ICOLUM,ICOLUM)
  320 DETERM=DETERM*PIVOT(I)
C
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
  330 A(ICOLUM,ICOLUM)=1.0
  340 DO 350 L=1,N
  350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT(I)
  355 IF(M)380,380,360
  360 DO 370 L=1,M
  370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT(I)
C
C     REDUCE NON-PIVOT ROWS
C
  380 DO 550 L1=1,N
  390 IF(L1-ICOLUM) 400,550,400
  400 T=A(L1,ICOLUM)
  420 A(L1,ICOLUM)=0.0
  430 DO 450 L=1,N
  450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
  455 IF(M) 550,550,460
  460 DO 500 L=1,M
  500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
  550 CONTINUE
C
C     INTERCHANGE COLUMNS
C
  600 DO 710 I=1,N
  610 L=N+1-I
  620 IF (INDEX(L,1)-INDEX(L,2)) 630,710,630
  630 JROW=INDEX(L,1)
  640 JCOLUM=INDEX(L,2)
  650 DO 705 K=1,N
  660 SWAP=A(K,JROW)
  670 A(K,JROW)=A(K,JCOLUM)
  700 A(K,JCOLUM)=SWAP
  705 CONTINUE
  710 CONTINUE
      GO TO 740
  739 DETERM=0.0
```

```
740 RETURN
750 END
```

```
@I FOR NOLIN
      SUBROUTINE NOLIN(X,N,EPS,EQS,PARTL)
      COMMON/FUNC/F(50),CK(50),CT(10)
      COMMON /GRAD/PD(50,50),AS(50,50),SQ(50)/RESID/GS(50)
      DIMENSION X(1),DELT(50)
      DOUBLE PRECISION F,CK,CT,PD,AS,SQ,GS
      DOUBLE PRECISION X,DELT,PHI,PH1,PH2
      EPS=1.E-3
      DL=1.E-8
      PH1=PHI(X,EQS)
C
   10 CONTINUE
      PH2=PH1
      CALL ASTAR(X,PARTL)
      CALL GSTAR(X,EQS)
      CALL DELTA(DELT,DL)
      IC=1
      DO 9 I=1,N
      TE=ABS(DELT(I))/(.001+ABS(X(I)))
      IF(TE.GT.EPS) IC=0
      X(I)=X(I)+DELT(I)
    9 CONTINUE
      IF(IC.EQ.1) RETURN
      PH1=PHI(X,EQS)
      IF(PH1.LT.1.D-7) DL=0.
      GO TO 10
      END
```

```
∂I FOR PHI
      FUNCTION PHI(X,EQS)
      DOUBLE PRECISION PHI,TEMP
      DOUBLE PRECISION F,CK,CT,X
C ***********************************************************************
C *     FORM THE SUM OF THE SQARES OF THE N FUNC.
C ***********************************************************************
      COMMON/FJNC/F(50),CK(50),CT(10)
      COMMON /LIMS/NF
      DIMENSION X(1)
      CALL EQS(X)
      TEMP=0.
      DO 1 I=1,NF
      TEMP=TEMP+F(I)*F(I)
    1 CONTINUE
      PHI=TEMP
      RETURN
      END
```

```
BI FOR FNEG
      FUNCTION FNEG(F,X)
      DOUBLE PRECISION FNEG,F,X
      IF(F.LT.0..AND.X.LT.-30.) GO TO 1
      FNEG=F
      RETURN
    1 CONTINUE
      X=X-1
      IF(X.LT.-85.) X=-85.
      FNEG=0.
      RETURN
      END
```

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